QUANTUM KINETIC THEORY: THE DISORDERED ELECTRON PROBLEM

T.R.KIRKPATRICK

Institute for Physical Science and Technology, and Department of Physics
University of Maryland, College Park, MD 20742

AND

D.BELITZ

Department of Physics and Materials Science Institute,University of Oregon,Eugene, OR 97403

Abstract. These are notes for lectures delivered at the NATO ASI on Dynamics in Leiden, The Netherlands, in July 1998. The quantum kinetic theory for noninteracting electrons in a disordered solid is introduced and discussed. We first use many-body theory to derive the quantum Boltzmann equation that describes transport and time correlation functions in this system. Particular attention is paid to the calculation of the electrical conductivity σ, and the density response function χ_{nn}. We then consider corrections to the Boltzmann equation due to wave interference effects. The disorder expansion of the conductivity is addressed, and the so-called weak localization or long-time tail contribution to σ is discussed. We conclude with a brief discussion of the influence of electron-electron interactions on the properties of disordered electronic systems.

Lectures delivered by T.R. Kirkpatrick

1. Introduction

Quantum kinetic theory has a long and interesting history. Shortly after the discovery of the Pauli exclusion principle, Sommerfeld applied it to electrons in metals and thereby resolved the most flagrant discrepancies between the observed thermal behavior of solids and the predictions of the classical Drude model of transport [1]. After the introduction of quantum mechanics, the new theory was incorporated into the standard Boltzmann description of transport. Like the classical Boltzmann equation, this quantum kinetic theory, also known as the Uhlenbeck-Uehling equation [2], is valid only for systems that are dilute in a sense to be explained below. Unlike the classical Boltzmann equation, it properly takes into account the statistics of the particles (fermionic or bosonic) as well as the quantum mechanical nature of the scattering process. However, it misses more subtle quantum mechanical effects. To get a feeling for what is missing, let us consider some length scales in the problem.

In a classical gas there are two length scales that occur in transport problems: The mean freee path ℓ, and the linear size of the particles or the impurities, which we denote by a. The Boltzmann transport theory is valid if the system is dilute in the sense that $a/\ell \ll 1$. In the quantum description of transport there is an additional length scale, namely the de Broglie wavelength λ of the scattered particle. Here we are interested in electron transport phenomena at temperatures that are low compared to the Fermi temperature, so the relevant length is λ_F, the de Broglie wavelength at the Fermi surface. Due to approximations made in its derivation, the quantum Boltzmann equation or Uhlenbeck-Uehling equation is only valid if both $a/\ell \ll 1$ and $\lambda_F/\ell \ll 1$. The latter expansion parameter indicates the relative importance of quantum mechanical wave interference effects.

In the first part of these lectures we introduce the standard Edwards model [3, 4] for noninteracting electrons in a disordered solid, and the two response functions that are most important for our purposes, viz. the electrical conductivity σ, and the density susceptibility $\chi_{nn}(\mathbf{k}, \omega)$. We then use simple kinetic theory concepts in conjunction with the particle number conservation law to show that the behavior of the latter at small frequencies ω and small wavevectors $\mathbf{k}$ is dominated by the hydrodynamic density diffusion mode. Simple arguments lead to an estimate for the value of the diffusion coefficient D in terms of the collision mean-free time τ. σ and D are related by an Einstein relation,

$$\sigma = e^2 \, \frac{\partial n}{\partial \mu} \, D \quad , \tag{1}$$

with e the electron change, n the electron number density, and μ the chemical potential. For noninteracting electrons at zero temperature, $\partial n/\partial \mu = N_{\mathrm{F}}$, with N_{F} the single particle density of states at the Fermi surface. Following this, we discuss how to derive the quantum Boltzmann equation and how to compute σ from it.

As mentioned above, the quantum Boltzmann equation is valid only in the 'semi-classical' limit where $\lambda_{\mathrm{F}}/\ell \to 0$. In the remaining parts of these lectures we discuss some of the interesting phenomena associated with wave interference that appear at higher order in an expansion in powers of $\sim \lambda_{\mathrm{F}}/\ell$. In particular, the nonanalytic nature of the disorder expansion of σ is discussed as well as weak-localization, or long-time tail, contributions to σ. We conclude with a few remarks on the combined effects of disorder and electron-electron interactions.

2. The model, and basic concepts

2.1. THE MODEL

We will be concerned with the electronic transport properties of disordered solids. In order to keep things simple, we will mainly consider a model that ignores the electron-electron interaction. While this approximation has yielded many important insights, one should keep in mind that in general it is not justified. We will come back to this point at the end of the lectures. For now we consider a noninteracting electron gas model consisting of spin $1/2$ fermions moving in a static random potential $u(\mathbf{x})$. Physically, $u(\mathbf{x})$ is produced by the impurities in the solid, and is therefore fixed for a given system, but we will assume that it is meaningful to consider an ensemble of systems and to compute averages of obervables over the random potential.[1] In the standard Edwards model [3, 4], $u(\mathbf{x})$ is taken to have zero mean, and to be Gaussian distributed with the variance given by,

$$\{u(\mathbf{x})u(\mathbf{y})\}_{\mathrm{dis}} = \frac{\delta(\mathbf{x} - \mathbf{y})}{2\pi N_{\mathrm{F}}\tau} \quad . \tag{2}$$

Here $N_{\mathrm{F}} = (m/2\pi)\,(k_{\mathrm{F}}/\pi)^{d-2}$ is the free electron density of states per spin at the Fermi surface (in $d = 2, 3$ dimensions), τ is the elastic mean-free time between collisions, $\{\ldots\}_{\mathrm{dis}}$ denotes the disorder average, k_{F} is the Fermi wavenumber, and m is the electron mass. Throughout the lectures we use units so that $\hbar = k_{\mathrm{B}} = e = 1$, with $\hbar$ Planck's constant, k_{B} Boltzmann's constant, and e minus the electron charge.

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[1]To what extent this assumption is justified is a very tricky question that we cannot get into. In principle one should calculate a whole distribution for every observable. Calculating the average is sufficient if this distribution is sharply peaked about its average.

To motivate this model we consider a quantum Lorentz gas, i.e. a system of moving electrons that interact with N stationary hard scatterers of radius a, but not with one another. The disorder average consists of averaging over the positions of the N scatterers in the system volume V, [2]

$$\{(\ldots)\}_{\text{dis}} = \frac{1}{V^N} \int d\mathbf{R}_1 \ldots d\mathbf{R}_N \, (\ldots) \quad , \tag{3}$$

and the electron-impurity potential can be written,

$$v(\mathbf{x}) = \sum_{i=1}^{N} v(\mathbf{x} - \mathbf{R}_i) \quad , \tag{4}$$

with $\{\mathbf{R}_i\}$ the positions of the N scatterers or impurities. Assuming that $\lambda(\approx \lambda_{\text{F}}) \gg a$, with a the s-wave scattering length, we can use a pseudo-potential [1] for a single electron-impurity interaction. In $d = 3$,

$$v(\mathbf{x} - \mathbf{R}_i) = \frac{4\pi a}{m} \delta(\mathbf{x} - \mathbf{R}_i) \quad . \tag{5}$$

The relevant scattering potential is given by $u(\mathbf{x}) = v(\mathbf{x}) - \{v(\mathbf{x})\}_{\text{dis}}$. Since the mean, $\{v(\mathbf{x})\}_{\text{dis}}$, simply redefines the Fermi energy, we can ignore it and have

$$\{u(\mathbf{x})u(\mathbf{y})\}_{\text{dis}} = \left(\frac{4\pi}{m}\right) a^2 \, n_i \, \delta(\mathbf{x} - \mathbf{y}) \quad . \tag{2'}$$

Here $n_i = N/V$ is the impurity density. Using $\tau \sim (n_i \, a^2)^{-1}$, in $d = 3$, we see that Eq. (2') has the same structure as Eq. (2). The reason for the other factors in Eq. (2) will become clear below.

Finally, we write down the Hamiltonian for the Edwards model in second quantization [4],

$$\hat{H} = \int d\mathbf{x} \, \hat{\psi}_\sigma^\dagger(\mathbf{x}) \left(-\frac{\nabla^2}{2m}\right) \hat{\psi}_\sigma(\mathbf{x}) + \int d\mathbf{x} \, u(\mathbf{x}) \, \hat{\psi}_\sigma^\dagger(\mathbf{x}) \, \hat{\psi}_\sigma(\mathbf{x}) \quad . \tag{6}$$

Here $\hat{\psi}_\sigma^\dagger$ and $\hat{\psi}_\sigma$ are fermion creation and annihilation operators with σ denoting a spin label, and summation over repeated Greek labels is understood.

2.2. LINEAR DENSITY RESPONSE

A standard technique in nonequilibrium statistical mechanics is to apply an external field to equilibrium systems, and to calculate the response of

[2]Here we neglect correlations between the scatterers, which are not important for our purposes.

the system to this field [5]. By expanding in powers of the external field, nonequilibrium quantities can be related to equilibrium time correlation functions. For example, let us apply an electric field $\mathbf{E}$ to an electron gas and expand to linear order in the field. Using Ohm's law, $\mathbf{J} = \sigma \cdot \mathbf{E}$, which relates the induced current $\mathbf{J}$ to the field, we obtain the so-called Kubo formula for the frequency dependent conductivity [6],

$$\sigma(\omega) = -\frac{n_e\, e^2}{m\, i\omega} + \frac{1}{\omega V}\int\limits_0^\infty dt\; e^{i\omega t}\left\{\left\langle 0\left|\left[\hat{J}_x(t), \hat{J}_x(t=0)\right]\right|0\right\rangle\right\}_{\mathrm{dis}}\quad. \tag{7}$$

Here n_e is the electron density, $\hat{J}_x(t)$ is the total current operator at time t in the x-direction, $[\hat{a}, \hat{b}]$ denotes the commutator of operators $\hat{a}$ and $\hat{b}$, and $\langle 0|\ldots|0\rangle$ denotes a ground state quantum mechanical expectation value.

Similarly, if we apply a potential $\varphi(\mathbf{x}, t)$ that couples to the density, then the change in the electronic density, δn, is given by,

$$\delta n(\mathbf{k}, \omega) = \chi_{nn}(k, \omega)\,\varphi(\mathbf{k}, \omega)\quad, \tag{8}$$

with χ_{nn} the density response function and $k = |\mathbf{k}|$. $\chi_{nn}(k, \omega)$ depends on k rather than on $\mathbf{k}$ because of rotational invariance once the disorder average has been performed. It is the Fourier transform of the density-density correlation function

$$\chi_{nn}(\mathbf{x}, t) = \Theta(t)\left\{\left\langle 0\left|[\hat{n}(\mathbf{x}=0, t=0), \hat{n}(\mathbf{x}, t)]\right|0\right\rangle\right\}_{\mathrm{dis}}\quad. \tag{9}$$

Here $\hat{n}$ is the density operator.

Equations (7) and (9) are valid for arbitrary systems. For noninteracting systems, some simplifications apply. In particular, the remaining many-body aspect of the problem (i.e., the correlations due to the Pauli principle) can be factored out, and the problem can be reduced to one of a *single* particle moving in a random potential. Technically, this is possible because the field operators ($\hat{\psi}^\dagger$ and $\hat{\psi}$) can be expanded in an exact eigenstate basis in terms of creation and annihilation operators $\hat{a}^\dagger$ and $\hat{a}$. The net result is that the quantum mechanical averages in Eqs. (7), (9) factorize. For example, the real part of the conductivity can be written

$$\begin{aligned}\sigma'(\omega) \equiv \mathrm{Re}\,\sigma(\omega) \;=\; & \frac{e^2}{2\pi V m^2}\mathrm{Re}\int d\mathbf{p}\, d\mathbf{p}_1\, p_x\, p_{1x}\left[\left\{G^R(\mathbf{p}, \mathbf{p}_1, E_{\mathrm{F}} + \omega)\right.\right.\\ & \left.\times\, G^A(\mathbf{p}_1, \mathbf{p}, E_{\mathrm{F}})\right\}_{\mathrm{dis}}\\ & \left.-\left\{G^A(\mathbf{p}, \mathbf{p}_1, E_{\mathrm{F}} + \omega)\, G^A(\mathbf{p}_1, \mathbf{p}, E_{\mathrm{F}})\right\}_{\mathrm{dis}}\right]\quad, \tag{10}\end{aligned}$$

with

$$G^{R,A}(\mathbf{p}_1, \mathbf{p}, E) = \left\langle \mathbf{p} \left| \frac{1}{E - H \pm i0} \right| \mathbf{p}_1 \right\rangle \quad , \tag{11}$$

denoting retarded (R) and advanced (A) Green functions. $|\mathbf{p}\rangle$ denotes a single-particle plane wave state, and $\hat{H}$ is the single-particle Hamiltonian,

$$\hat{H} = -\frac{\nabla^2}{2m} + u(\mathbf{x}) \quad . \tag{12}$$

Similarly, the density response function can be written,

$$\chi_{nn}(k, \omega) = N_\mathrm{F} \; + \; \frac{i\omega}{2\pi} \int d\mathbf{p}\, d\mathbf{p}_1 \left\{ G^R(\mathbf{p} + \mathbf{k}, \mathbf{p}_1 + \mathbf{k}, E_\mathrm{F} + \omega) \right.$$
$$\left. \times\, G^A(\mathbf{p}_1, \mathbf{p}, E_\mathrm{F}) \right\}_{\mathrm{dis}} \quad . \tag{13}$$

2.3. SOME ADDITIONAL REMARKS

In the long-wavelength limit, the form of $\chi_{nn}(k, \omega)$ is determined by the diffusive nature of the electron dynamics in a disordered solid. This can be seens as follows. The conservation law for the particle number density is expressed by the continuity equation

$$\partial_t \, \delta n(\mathbf{x}, t) + \nabla \cdot \mathbf{j}(\mathbf{x}, t) = 0 \quad , \tag{14}$$

with $\mathbf{j}$ the number current density. In addition, Fick's law, valid in the long-wavelength limit, gives a relation between $\mathbf{j}$, δn, and φ,

$$\mathbf{j}(\mathbf{x}, t) = -D \, \nabla \delta n + \mu_\mathrm{e} \nabla \varphi \quad . \tag{15}$$

with D the diffusion coefficient and $\mu_\mathrm{e} = D\partial n/\partial\mu = DN_\mathrm{F}$ the electron mobility (not to be confused with the chemical potential μ). Using Eq. (15) in Eq. (14), performing a Fourier-Laplace transform, and comparing with Eq. (8) gives

$$\chi_{nn}(k, \omega) = \frac{N_\mathrm{F} D k^2}{-i\omega + Dk^2} \quad . \tag{16}$$

The above arguments tell us the functional form of χ_{nn} in the long-wavelength small-frequency limit, but they do not tell us the value of the diffusivity D. Rather, D enters as a purely phenomenological quantity. However, we can get a rough idea of the value of D, and of the closely related conductivity, by means of simple dimensional analysis. The units of D are L^2/T, with L a length scale and T a time scale. There are three length scales in the problem: The Fermi wavelength λ_F, the scattering length a, and the

scattering mean-free path ℓ. Clearly, the relevant length for transport processes is ℓ. Similarly, the relevant time scale is the scattering mean-free time τ. For electrons on the Fermi surface, $\ell = v_\mathrm{F}\tau$, with $v_\mathrm{F} = k_\mathrm{F}/m$ the Fermi velocity. As an order of magnitude estimate of D we therefore expect

$$D \simeq v_\mathrm{F}^2 \tau \quad . \tag{17}$$

Using Eq. (1) and $v_\mathrm{F}^2 N_\mathrm{F} \simeq n_e/m$, the analogous estimate for the conductivity σ is

$$\sigma \simeq \frac{n_e e^2 \tau}{m} \quad . \tag{18}$$

This is the standard Drude result for σ.

Clearly, all of the above arguments and derivations are just phenomenological in nature, and therefore ultimately unsatisfactory, although they do contain the correct physics. In the following section we improve our treatment, and derive the Eqs. (16), (17), and (18) from the microscopic Hamiltonian.

3. Many Body Perturbation Theory

3.1. THE DISORDER AVERAGED GREEN FUNCTION

For pedagogical reasons, let us first calculate the averaged Green function, although it is not directly needed to compute either Eq. (10) or Eq. (13). Since on average space is homogeneous, we have

$$\left\{ G^{R,A}(\mathbf{p}, \mathbf{p}_1, E) \right\}_\mathrm{dis} = \delta(\mathbf{p} - \mathbf{p}_1)\, G^{R,A}(\mathbf{p}, E) \quad . \tag{19}$$

A self-energy Σ can be defined in the usual way, leading to a Dyson equation for the Green function [5]. To be specific, we consider the retarded Green function,

$$\begin{aligned} G^R(\mathbf{p}, E) &= G_0^R(\mathbf{p}, E) + G_0^R(\mathbf{p}, E)\, \Sigma^R(\mathbf{p}, E)\, G^R(\mathbf{p}, E) \\ &= \frac{1}{E - \mathbf{p}^2/2m - \Sigma^R(\mathbf{p}, E) + i0} \quad , \end{aligned} \tag{20}$$

with G_0 the free particle Green function (i.e., Eq. (20) with $\Sigma^R = 0$).

Standard methods lead to a diagrammatic theory for Σ^R [3]. In Fig. 1 (a), we show the lowest order, or Born, approximation for the self-energy. Here the straight line denotes a free particle Green function and the dashed line with a cross denotes a $\{u\,u\}_\mathrm{dis}$ disorder correlation function. In this
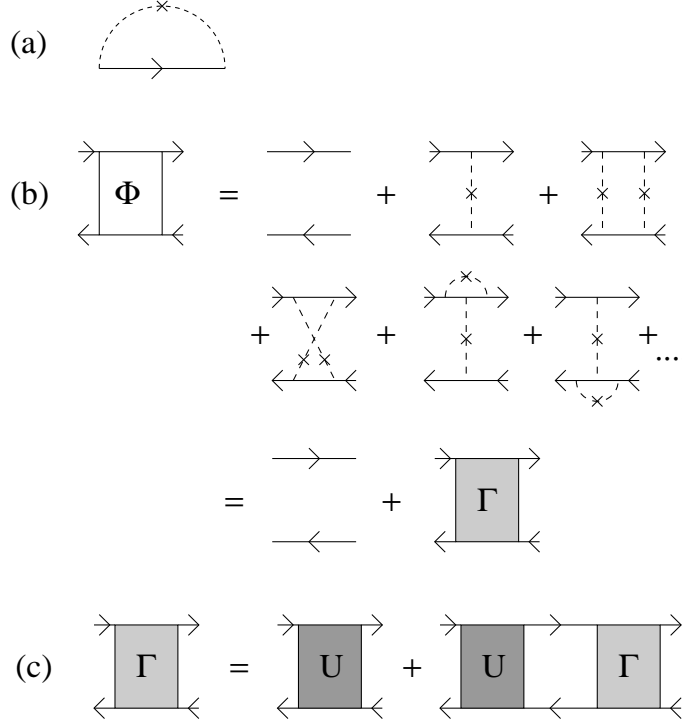
Figure 1. (a) Born approximation for the electron self-energy. (b) Perturbation theory for the two-particle correlation function Φ, Eq. (23). (c) The reducible vertex function Γ in terms of the irreducible vertex function U.

approximation,

$$\Sigma^R(\mathbf{p}, E) = \frac{1}{2\pi N_F \tau} \int_{\mathbf{q}} \frac{1}{[E - q^2/2m + i0]} \approx \frac{-i\pi}{2\pi N_F \tau} \int_{\mathbf{q}} \delta\left(E - \frac{q^2}{2m}\right)$$

$$= -\frac{i}{2\tau} \quad , \tag{21}$$

Here $\int_{\mathbf{q}} \equiv \int d\mathbf{q}/(2\pi)^d$, and we have dropped the real part of Σ^R, which simply redefines the zero of the energy. In this approximation the average Green function is,

$$G^R(\mathbf{p}, E) \approx \frac{1}{E - \mathbf{p}^2/2m + i/2\tau} \quad . \tag{22}$$

We see that the factors in Eq. (2) were chosen so that the time Fourier transform of Eq. (22), $G^R(\mathbf{p}, t)$, decays exponentially with a relaxation

time equal to τ. The physical meaning of this decay is the loss of phase correlations that is brought about by the electron-impurity scattering.

3.2. THEORY FOR THE CONDUCTIVITY AND THE DENSITY SUSCEPTIBILITY: GENERALIZED BOLTZMANN EQUATION

In order to calculate the conductivity and the density susceptibility, Eqs. (10) and (13), we introduce the two-particle correlation function,

$$\Phi_{\mathbf{pp}_1}(\mathbf{k},\omega) = \left\{ G^R\left(\mathbf{p}+\mathbf{k},\mathbf{p}_1+\mathbf{k},E_F+\omega\right) G^A\left(\mathbf{p}_1,\mathbf{p},E_F\right) \right\}_{\text{dis}} \quad . \quad (23)$$

The advanced-advanced combination $G^A G^A$ also contributes to Eq. (10), but it is not important for the effects we are interrerested in and we therefore do not dicuss it.

A diagrammatic expression for Φ is shown in Fig. 1 (b). Here the straight lines denote exact averaged Green functions, and the shaded box indicates disorder correlations between the top (retarded) and bottom (advanced) Green functions. A Bethe-Salpeter equation can be used to introduce a two-particle irreducible vertex, $U_{\mathbf{pp}_1}$, which is the two-particle analog of the Dyson self-energy. The diagrammatic relationship between the reducible vertex Γ, and the irreducible one is shown in Fig. 1 (c). Analytically we have

$$\begin{aligned}
\Phi_{\mathbf{pp}_1}(\mathbf{k},\omega) \quad = \quad & G^R\left(\mathbf{p}+\mathbf{k},E_F+\omega\right) G^A\left(\mathbf{p},E_F\right) \Big[\delta(\mathbf{p}-\mathbf{p}_1) \\
& + \int_{\mathbf{p}_2} U_{\mathbf{pp}_2}(\mathbf{k},\omega)\Phi_{\mathbf{p}_2\mathbf{p}_1}(\mathbf{k},\omega) \Big] . \quad (24)
\end{aligned}$$

To put this into a more standard form we write [7],

$$G^R\left(\mathbf{p}+\mathbf{k},E_F+\omega\right) G^A\left(\mathbf{p},E_{rmF}\right) = -\frac{\Delta G_{\mathbf{p}}(\mathbf{k},\omega)}{\omega - \mathbf{k}\cdot\mathbf{p}/m - \Delta\Sigma_{\mathbf{p}}(\mathbf{k},\omega)} \quad , \quad (25)$$

where
$$\Delta G_{\mathbf{p}}(\mathbf{k},\omega) = G^R\left(\mathbf{p}+\mathbf{k},E_F+\omega\right) - G^A\left(\mathbf{p},E_F\right) \quad , \quad (26)$$

$$\Delta\Sigma_{\mathbf{p}}(\mathbf{k},\omega) = \Sigma^R(\mathbf{p}+\mathbf{k},E_F+\omega) - \Sigma^A(\mathbf{p},E_F) \quad . \quad (27)$$

Defining $\widetilde{\Phi}$ through

$$\Phi_{\mathbf{pp}_1}(\mathbf{k},\omega) = \Delta G_{\mathbf{p}}(\mathbf{k},\omega)\, \widetilde{\Phi}_{\mathbf{pp}_1}(\mathbf{k},\omega) \quad , \quad (28)$$

and using the Ward identity [7],

$$\Delta\Sigma_{\mathbf{p}}(\mathbf{k},\omega) = \int_{\mathbf{p}_2} U_{\mathbf{pp}_2}(\mathbf{k},\omega)\, \Delta G_{\mathbf{p}_2}(\mathbf{k},\omega) \quad , \quad (29)$$

the Eq. (24) can be written,

$$\left\{\omega - \frac{\mathbf{k}\cdot\mathbf{p}}{m}\right\}\widetilde{\Phi}_{\mathbf{p}\mathbf{p}_1}(\mathbf{k},\omega) \;=\; -\delta(\mathbf{p}-\mathbf{p}_1) + \int_{\mathbf{p}_2} U_{\mathbf{p}\mathbf{p}_2}(\mathbf{k},\omega)\,\Delta G_{\mathbf{p}_2}(\mathbf{k},\omega)$$
$$\times\left[\widetilde{\Phi}_{\mathbf{p}\mathbf{p}_1}(\mathbf{k},\omega) - \widetilde{\Phi}_{\mathbf{p}_2\mathbf{p}_1}(\mathbf{k},\omega)\right] \quad . \;(30)$$

Two comments are in order. First, for small wavevectors and frequencies,

$$\Delta G_{\mathbf{p}}(\mathbf{k}\to 0, \omega\to 0) \approx -i\pi\delta(E - p^2/2m)/\tau \quad ,$$

so that the ΔG in Eqs. (30) and (25) are delta-functions that confine the electrons to the energy shell. Second, Eq. (30) for Φ is exact, and has the form of a generalized Boltzmann equation. That is, the frequency term on the left hand side is the Fourier transform of a time derivative, and $\mathbf{k}\cdot\mathbf{p}/m$ is the spatial Fourier transform of $\mathbf{p}\cdot\nabla/m$. Therefore the left-hand side has the form of a standard free-streaming term. The right-hand side, on the other hand, is an initial condition term, plus a generalized collision operator. In the next subsection, we will see that the simplest approximation for U leads to the quantum Boltzmann equation.

In terms of $\widetilde{\Phi}$, the physical quantities of interest to us are

$$\sigma'(\omega) = \frac{e^2}{2\pi V m^2}\int d\mathbf{p}\,d\mathbf{p}_1\,p_x\,p_{1x}\,\Delta G_{\mathbf{p}}(\mathbf{0},\omega)\,\widetilde{\Phi}_{\mathbf{p}\mathbf{p}_1}(\mathbf{0},\omega) \quad , \qquad (31)$$

and

$$\chi_{nn}(k,\omega) = N_{\mathrm{F}} + \frac{i\omega}{2\pi}\int d\mathbf{p}\,d\mathbf{p}_1\,\Delta G_{\mathbf{p}}(\mathbf{k},\omega)\,\widetilde{\Phi}_{\mathbf{p}\mathbf{p}_1}(\mathbf{k},\omega) \quad . \qquad (32)$$

3.3. QUANTUM BOLTZMANN EQUATION

To lowest order in the disorder we have, cf. Fig. 2,

$$U_{\mathbf{p}\mathbf{p}_2}(\mathbf{k},\omega) = \frac{i}{2\pi N_{\mathrm{F}}\tau} \quad . \qquad (33)$$
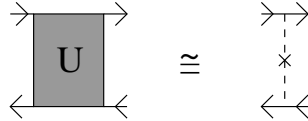
Inserting Eqs. (33) in Eq. (30) yields,

Figure 2.   Boltzmann approximation for the irreducible vertex function U.

$$\left\{-i\omega + i\frac{\mathbf{k}\cdot\mathbf{p}}{m}\right\}\widetilde{\Phi}_{\mathbf{pp}_1}(\mathbf{k},\omega) \;=\; i\delta(\mathbf{p}-\mathbf{p}_1) + \frac{1}{N_{\mathrm{F}}\tau}\int\limits_{\mathbf{p}_2}\delta(E_{\mathrm{F}} - p_2^2/2m)$$
$$\times\left[\widetilde{\Phi}_{\mathbf{p}_2\mathbf{p}_1}(\mathbf{k},\omega) - \widetilde{\Phi}_{\mathbf{pp}_1}(\mathbf{k},\omega)\right]. \quad (34)$$

This is the quantum Boltzmann equation, which thus turns out to be the simplest nontrivial approximation within the formalism developed above. Higher order approximations for $U_{\mathbf{pp}_2}$ lead to corrections of order $\lambda_{\mathrm{F}}/\ell$ and a/ℓ to the Boltzmann equation results.

The Eq. (34) can be easily solved exactly. One obtains,

$$\widetilde{\Phi}_{\mathbf{pp}_1}(\mathbf{k},\omega) \;=\; i\delta(\mathbf{p}-\mathbf{p}_1)\,h_{\mathbf{p}}(\mathbf{k},\omega)$$
$$+\frac{i\,\delta(E_{\mathrm{F}} - p_1^2/2m)\,h_{\mathbf{p}}(\mathbf{k},\omega)}{N_{\mathrm{F}}\tau\left[1 - \frac{1}{N_{\mathrm{F}}\tau}\int\limits_{\mathbf{p}_2}\delta(E_{\mathrm{F}} - p_2^2/2m)\,h_{\mathbf{p}_2}(\mathbf{k},\omega)\right]}\quad, \quad (35)$$

with

$$h_{\mathbf{p}_2}(\mathbf{k},\omega) = \left(-i\omega + i\frac{\mathbf{k}\cdot\mathbf{p}}{m} + \frac{1}{\tau}\right)^{-1}. \quad (36)$$

For general $\mathbf{k}$ and ω, Eq. (35) is quite complicated. However, using it in Eqs. (31) and (32) for small wavenumber and frequency immediately gives

$$\sigma_{\mathrm{B}} = n_e\frac{e^2\tau}{m}\quad, \quad (37)$$

and,

$$\chi_{nn,\mathrm{B}}(\mathbf{k},\omega) \simeq \frac{N_{\mathrm{F}}D_{\mathrm{B}}k^2}{-i\omega + D_{\mathrm{B}}k^2}\quad, \quad (38)$$

where the subscript B denotes the Boltzmann approximation. Notice that σ_{B} and D_{B} are related by the Einstein relation,

$$\sigma_{\mathrm{B}} = e^2 N_{\mathrm{F}}D_{\mathrm{B}}\quad, \quad (39)$$

as they should be according to Eq. (1).

4. Corrections to Boltzmann Transport Theory: Wave Interference Effects

4.1. DISORDER OR DENSITY EXPANSION OF σ

Perhaps the most obvious theoretical problem concerning the wave interference effects is to characterize the corrections to σ_B that arise when $\lambda_{\mathrm{F}}/\ell$ is not zero. The first question is whether or not there is an analytic expansion

in the small parameter $\epsilon = \lambda_F/\ell$. Technically, this question can be answered by examining the coefficients a_i $(i = 1, 2, 3, \ldots)$ in the Taylor expansion,

$$\frac{\sigma}{\sigma_B} = 1 + a_1\, \epsilon + a_2\, \epsilon^2 + O(\epsilon^3) \quad . \tag{40}$$

Detailed calculations show that in general such an expansion does not exist, and that all the coefficients beyond a_{d-1} are infinite in d dimensions [8]. Although of different physical origin, a similar divergence is well known to exist in the kinetic theory of classical gases [9].
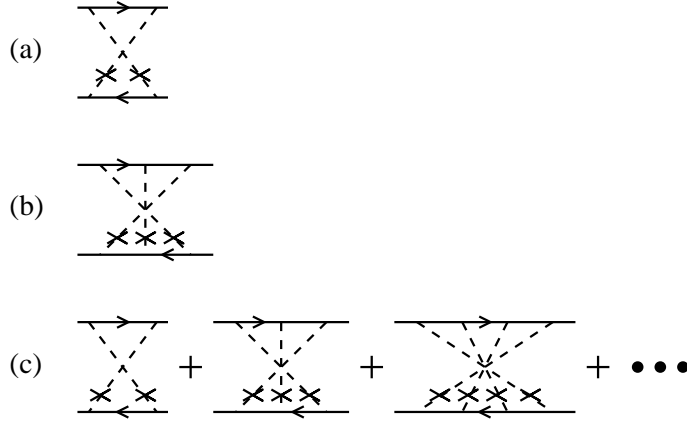
(a)

(b)

(c)

Figure 3.   Maximally crossed diagrams.

To see the origin of these infinities in the quantum case, consider the first few maximally crossed diagrams (MCD) in Fig. 3. The calculation gives,

$$(3a) \propto \int_q G^R(\mathbf{q})\, G^A(\mathbf{p} + \mathbf{p}_1 - \mathbf{q})\Big|_{\omega=1/\tau=0} \propto \frac{1}{|\mathbf{p} + \mathbf{p}_1|} \tag{41}$$

$$(3b) \propto (3a)^2 \propto \frac{1}{|\mathbf{p} + \mathbf{p}_1|^2} \quad . \tag{42}$$

That is, the MCD are singular for the momentum configuration that corresponds to backscattering, $\mathbf{p}_1 = -\mathbf{p}$. In any dimension, these singularities lead to infinite coefficients in Eq. (40), with the order in which the first infinity occurs depending on the dimension. The correct expansion of σ in powers of ϵ is therefore nonanalytic. In $d = 3$, it is of the form

$$\frac{\sigma}{\sigma_B} = 1 + a_1\, \epsilon + a_2'\, \epsilon^2 \ln 1/\epsilon + a_2\, \epsilon^2 + \ldots \quad . \tag{43}$$

In $d = 2$ it has been shown that power-law nonanalyticities appear in addition to logarithmic ones [10]. In the next subsection we further discuss the backscattering processes that cause these nonanalyticities.

For most systems, the values of the coefficients in Eq. (43) are of limited interest because the derivation has ignored electron-electron interactions, which are important in all solid state materials. However, there does exist a physical system for which the quantum Lorentz gas is a realistic model, namely electrons injected into He gas at low ($\leq 4°$K) temperatures. In Ref. [11] detailed arguments have been given that on electronic time scales, the He atoms can be treated as stationary scatterers and that all other approximations used in our model are justified for describing transport in this system. The finite temperature electron mobility, μ, normalized to its Boltzmann value, can be expanded in the small parameter

$$\chi = \lambda_T/\pi\ell \quad , \tag{44}$$

with $\lambda_T \equiv 2\pi/k_T = \sqrt{2\pi^2/mT}$ the thermal de Broglie wavelength. The result is,

$$\frac{\mu}{\mu_B} = 1 + \mu_1\,\chi + \mu_2'\,\chi^2\ln\chi + \mu_2\,\chi^2 + \dots \quad , \tag{45}$$

with,

$$\begin{aligned}
\mu_1 &= -\pi^{3/2}/6 \quad , \\
\mu_2' &= (\pi^2 - 4)/32 \quad , \\
\mu_2 &= 0.236 \quad .
\end{aligned} \tag{46}$$

In Fig. 4 this theoretical result, with no adjustable parameters, is compared to experimental data. We conclude that experiments are consistent with Eqs. (45) and (46). Further experiments are needed to unambigiously confirm the presence of the logarithm in these equations. For further discussions of this point, see Ref. [11].

4.2. WEAK LOCALIZATION EFFECTS AND LONG-TIME TAILS

In classical transport theory it has proven to be very enlightening to examine the long-time properties of the time correlation functions (TCF) that determine the transport coefficients. Generally, it has been found that these functions decay algebraically for long times and that therefore the transport coefficients themselves are nonanalytic functions of the frequency [9]. In quantum transport theory the decay of the TCF has proven to be even more interesting [13], and to be closely related to the phenomenon of Anderson localization [14]. Note that in either case, these algebraic tails are qualitatively different from the exponential decays predicted by both the Boltzmann equation and by simple theories for the Green function.
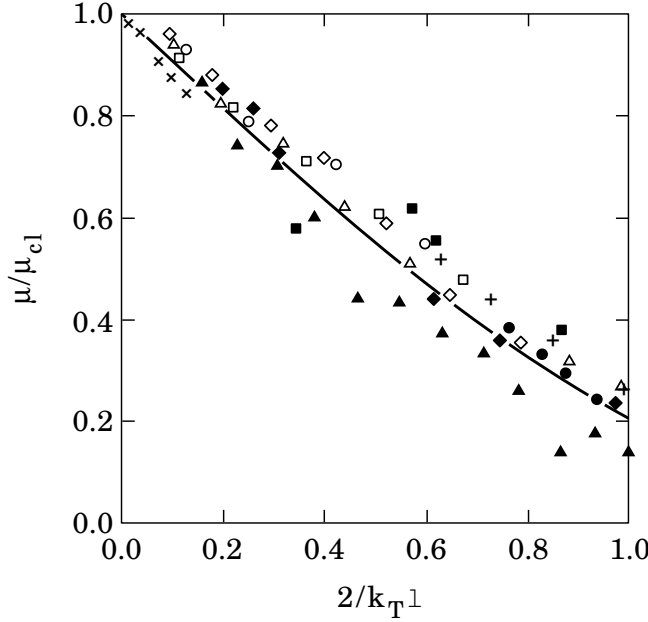
Figure 4.   Mobility μ of electrons in dense gases, normalized to the Boltzmann value μ_{cl}, as a function of χ. The symbols represent experimental data as measured or quoted by Adams at al. [12]. The solid line is the theoretical result, Eqs. (45,46). From Ref. [13].

Here we mainly concentrate on a physical argument [15] that leads to these so-called weak localization effects. Some hints of their technical origin will also be given; details can be found elsewhere [14]. We will see that the weak localization effects are closely related to the same backscattering phenomena that are responsible for the nonanalytic disorder expansion discussed in the previous subsection.

The physical argument starts by considering the different Feynman paths from, say, point A to point B, as illustrated in Fig. 5. Labeling the amplitude of path i by $\mathcal{A}_i$, the total probability to reach B from A is,

$$w = \left| \sum_i \mathcal{A}_i \right|^2 = \sum_i |\mathcal{A}_i|^2 + \sum_{i \neq j} \mathcal{A}_i \, \mathcal{A}_j^* \quad . \tag{47}$$

Usually, the different paths are uncorrelated and the second term in Eq. (47) averages to zero, leaving the first term, which is just the classical probability. The exception to this is if the points A and B coincide. In this case the path can be traversed in two opposite directions, namely, forward or backward. The amplitudes $\mathcal{A}_1$ and $\mathcal{A}_2$ for these two paths have a coherent phase relation, leading to constructive interference. If $\mathcal{A}_1 = \mathcal{A}_2 = \mathcal{A}$, then
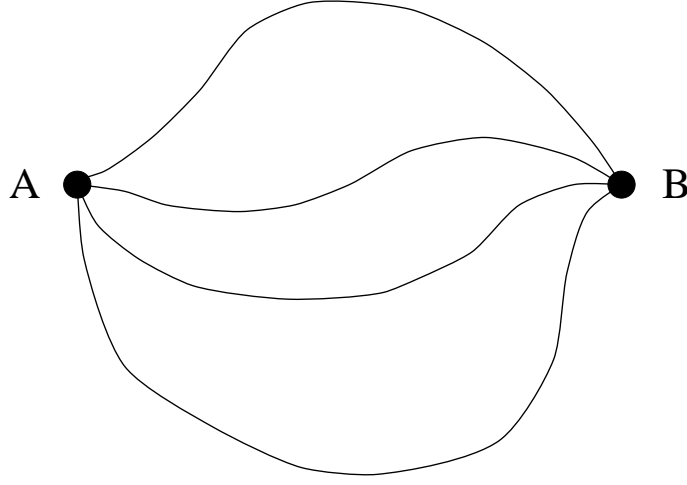
Figure 5.   Feynman paths from point A to point B.

Eq. (47), for $i = 1, 2$, becomes

$$w = 2 \, |\mathcal{A}|^2 + 2\mathcal{A} \, \mathcal{A}^* = 4 \, |\mathcal{A}|^2 \quad , \tag{47'}$$

which is twice the classical probability. The important conclusion from this argument is that the quantum probabilities for time reversed, or intersecting, paths are enhanced compared to classical dynamics. Further, since paths that return to their starting point slow down the diffusion process, we expect these quantum corrections to lead to a decrease of σ compared to the semi-classical value.

   To estimate the contribution of the closed loops to σ we argue as follows. If the particle is diffusing, then the probability of finding it at point $\mathbf{r}$ at time t, given that it was at point $\mathbf{r}_0$ at time $t = 0$ is

$$w(\mathbf{r}, t) = \frac{\exp[-(\mathbf{r} - \mathbf{r}_0)^2 / 4Dt]}{(4\pi Dt)^{d/2}} \quad , \tag{48}$$

$w(\mathbf{r}, t)$ is appreciably different from zero only within a diffusive volume V_{diff} determined by $(\mathbf{r} - \mathbf{r}_0)^2 < 4Dt$, or,

$$V_{\text{diff}} \approx (Dt)^{d/2} \quad . \tag{49}$$

 Now, each Feynman path has a diameter proportional to λ_{F}^{d-1}, and a differential length $d\ell = v_{\text{F}} \, dt$, cf. Fig. 6. The differential volume of the
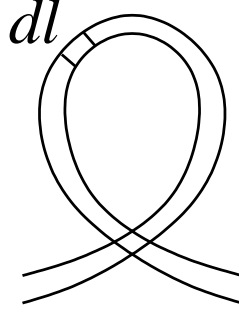
Figure 6.   Geometry of a Feynman tube.

Feynman tube is $dV = V_\mathrm{F}\lambda_p^{d-2}dt$, which should be compared to V_diff. If p is the probability that a closed path exists, then it is the ratio of these two volumes integrated over all times:

$$p = \int_{\tau'}^{T} \frac{dV}{V_\mathrm{diff}} = \lambda_\mathrm{F}^{d-1}v_\mathrm{F} \int_{\tau'}^{T} \frac{dt}{(Dt)^{d/2}} \quad . \tag{50}$$

Here $\tau' = O(\tau)$ is a microscopic time where the diffusive description breaks down, and T is the observation time that we will equate with w^{-1}. The change in $\delta\sigma$ of the conductivity due to these wave interference effects is therefore,

$$\frac{\delta\sigma}{\sigma_0} \propto - \begin{cases} 1/(\omega\tau)^{1/2} & , \quad (d=1) \\ \ln(1/\omega\tau) & , \quad (d=2) \\ \mathrm{const.} - (\omega\tau)^{1/2} & , \quad (d=3) \end{cases} \quad . \tag{51}$$

Note that the low frequency correction to σ_0 in Eq. (51) diverges as $\omega \to 0$ for $d \leq 2$. Further, these contributions have a sign such as to decrease the conductivity. In a more complete theory that effectively resums all such divergent contributions, σ is identically equal to zero for $\omega = 0$ in $d \leq 2$ [14]. This phenomenon is known as Anderson localization. In $d > 2$ a metal-insulator transition, called the Anderson transition, occurs as a function of the disorder or the Fermi energy. In $d = 2$ there cannot be a metallic phase, as the electrons are always localized. $d = 2$ is therefore the lower critical dimension for the Anderson transition.

The same results can also be obtained from the generalized Boltzmann equation derived in Sec. 3. Resumming all of the backscattering or MCD diagrams shown in Fig. 3 leads to Eq. (51) with explicit coefficients. The crucial point is that the summations of the MCD can be related, in the absence of a magnetic field, to the summation of ladder diagrams that give

χ_{nn}. Analytically, the MCD lead to a contribution of the form

$$\frac{\delta\sigma}{\sigma_0} \approx -c_d \int\limits_{q<\ell^{-1}} \frac{1}{-i\omega + D_{\mathrm{B}}q^2} \quad . \tag{52}$$

Here $\mathbf{q} = \mathbf{p} + \mathbf{p}_1$ is the backscattering momentum, a long-wavelength approximation has been made so that $q < \ell^{-1}$, and $c_d \sim \lambda_{\mathrm{F}}^{d-1}$ is a constant. Performing the integral gives Eq. (51). At finite temperatures the ω in Eq. (51) is effectively replaced by T (see below), so that σ depends nonanalytically, and in $d = 1, 2$ singularly, on T. In Fig. 7, the resistivity $\rho \sim 1/\sigma$ is plotted versus $\ln 1/T$ for a two-dimensional amorphous film. The straight line confirms the existence of the logarithm in Eq. (51).
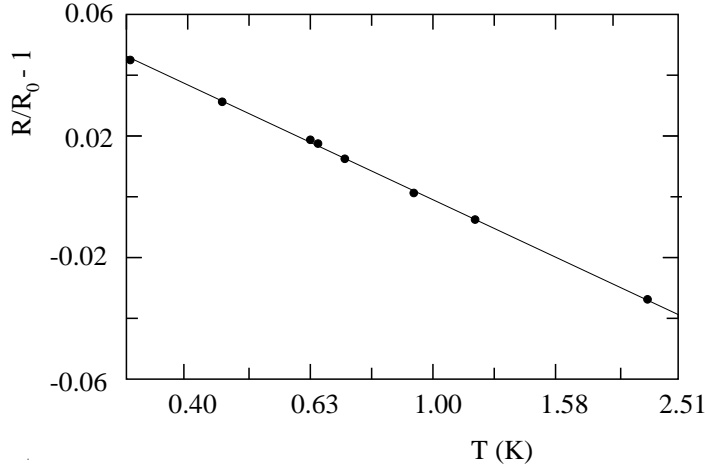

Figure 7. Resistance, R, normalized to $R_0 = R(T = 1K)$, of a thin PdAu film plotted versus $\log T$ as measured by Dolan and Osheroff [16]. From Ref. [13].

It is worth noting that the hydrodynamic pole in Eq. (52) occurs because the MCD are related to a spontaneously broken symmetry and a corresponding Goldstone mode [17]. This mode is soft or massless only at zero temperature. That is, the relationship of the MCD to χ_{nn} that was noted above, is valid only for $T = 0$. At finite temperature, the ω in Eq. (52) is replaced by $\omega + 1/\tau_{\mathrm{in}}$, with τ_{in} the temperature dependent inelastic mean-free time. The Goldstone modes thus acquire a mass, in contrast to χ_{nn} which is always massless due to particle number conservation. In the literature, in analogy to particle physics terminology, these modes that are hydrodynamic only at $T = 0$ are often called either 'diffusons' or 'Cooperons', depending on how they arise.

4.3. THE EFFECTS OF ELECTRON-ELECTRON INTERACTIONS

In the absence of electron-electron interactions it is easy to show that thermodynamic quantities do not depend on the dynamical diffusive processes that lead to the low frequency nonanalyticities discussed in the previous subsection. However, when interactions are included this is no longer the case, and the static and dynamical properties of any quantum system are coupled together. From a technical point of view this is obvious within a many-body Matsubara formalism. From a scaling viewpoint, in fundamental units ($\hbar = 1 = k_{\mathrm{B}}$) T and ω have the same units, implying thermodynamics (T) and dynamics (ω) are coupled together.

   To motivate the static results, we note that for diffusive systems, ω scales like k^2. For the wavenumber and frequency dependent conductivity this implies, for $2 < d < 4$,

$$\frac{\sigma(k = 0, \omega)}{\sigma_0} = 1 + a\,\omega^{(d-2)/2} + \dots \quad , \tag{53}$$

$$\frac{\sigma(k, \omega = 0)}{\sigma_0} = 1 + a'\,k^{d-2} + \dots \quad . \tag{54}$$

Note that the coefficients a and a' in Eqs. (4.3) are positive since wave interference effects decrease $\sigma(0,0)$. Another interesting quantity is the static spin susceptibility, $\chi_s(k)$, as a function of the wavenumber. Disorder slows down the electrons, so that in effect any two electrons spend more time close to one another, i.e., disorder effectively increases the strength of the electron-electron interactions. This in turn implies a disorder induced increase in χ_s. Calculations similar to those that lead to Eqs. (53), (54) give, at $T = 0$ [18],

$$\frac{\chi_s(k)}{\chi_s(0)} = 1 - \widetilde{a}\,k^{d-2} + 0(k^2) \quad . \tag{55}$$

In real space, this in turn implies long-range equal-time spin correlations that decay like

$$\chi_s(r) \sim 1/r^{2(d-1)} \quad . \tag{56}$$

This is a remarkable result. In classical statistical mechanics, $\chi_s(r) \propto \exp(-r/\xi)$, with ξ the correlation length which, away from any critical point, is on the order of the lattice spacing. In contrast, at $T = 0$, the correlations in Eq. (55) are power-law like everywhere in the phase diagram. These long-range correlations are due to a coupling of the hydrodynamic spin transport to the charge diffusion processes which themselves are intrinsically of long range.

   Physically, Eq. (55) implies that spin fluctuations effectively interact between themselves through long-range interactions. It is well known that

long-range interactions have a profound effect on phase transitions and critical behavior. The implication of Eq. (55) for the paramagnetic to ferromagnetic quantum phase transition is discussed in the following lectures [19]. Note that long-range spatial correlations also exist in *nonequilibrium classical* systems. In that case, statics and dynamics are also coupled together, somewhat analogous to the *equilibrium quantum* statistical mechanical systems discussed here [13].

5. Final Remarks

We conclude with a few additional remarks. Although we have not emphasized this fact, the interesting phenomena in quantum kinetic theory discussed above have strong analogies in classical kinetic theory. Indeed, the discovery of the logarithmic singularity in the disorder expansion of σ, Eq. (43), was motivated by much earlier, related considerations in classical kinetic theory [9]. Similarly, long-time tail effects and low-frequency nonanalyticities were discussed already in 1967 for classical systems [21], whereas the weak localization effects discussed above were not discovered until 1979 [20].

Another aspect we have not stressed is that, even though the phenomena in classical and quantum systems are similar, the correlations in space and time are stronger in the quantum mechanical case. For example, in the classical Lorentz gas the low frequency nonanalytic contribution to the conductivity is proportional to $\omega^{d/2}$. Physically, this eventually leads to the conclusion that while classical particles are diffusive in $d = 2$, there is no diffusive phase in two-dimensional quantum systems [20, 14].

Finally, one other important feature in quantum systems is the coupling between statics and dynamics. In classical systems the thermodynamic correlation functions do not couple to the dynamical fluctuations that lead to the long-range correlations in time correlation functions. In zero temperature quantum systems the situation is different. As explained in the last section, equal time correlations do couple to these dynamical fluctuations, and as a consequence of this, there are both long-ranged, power-law spatial correlations and long-ranged, power-law time correlations in quantum systems.

Acknowledgements

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